Engine Research at LLNL

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Lawrence Livermore National Laboratory

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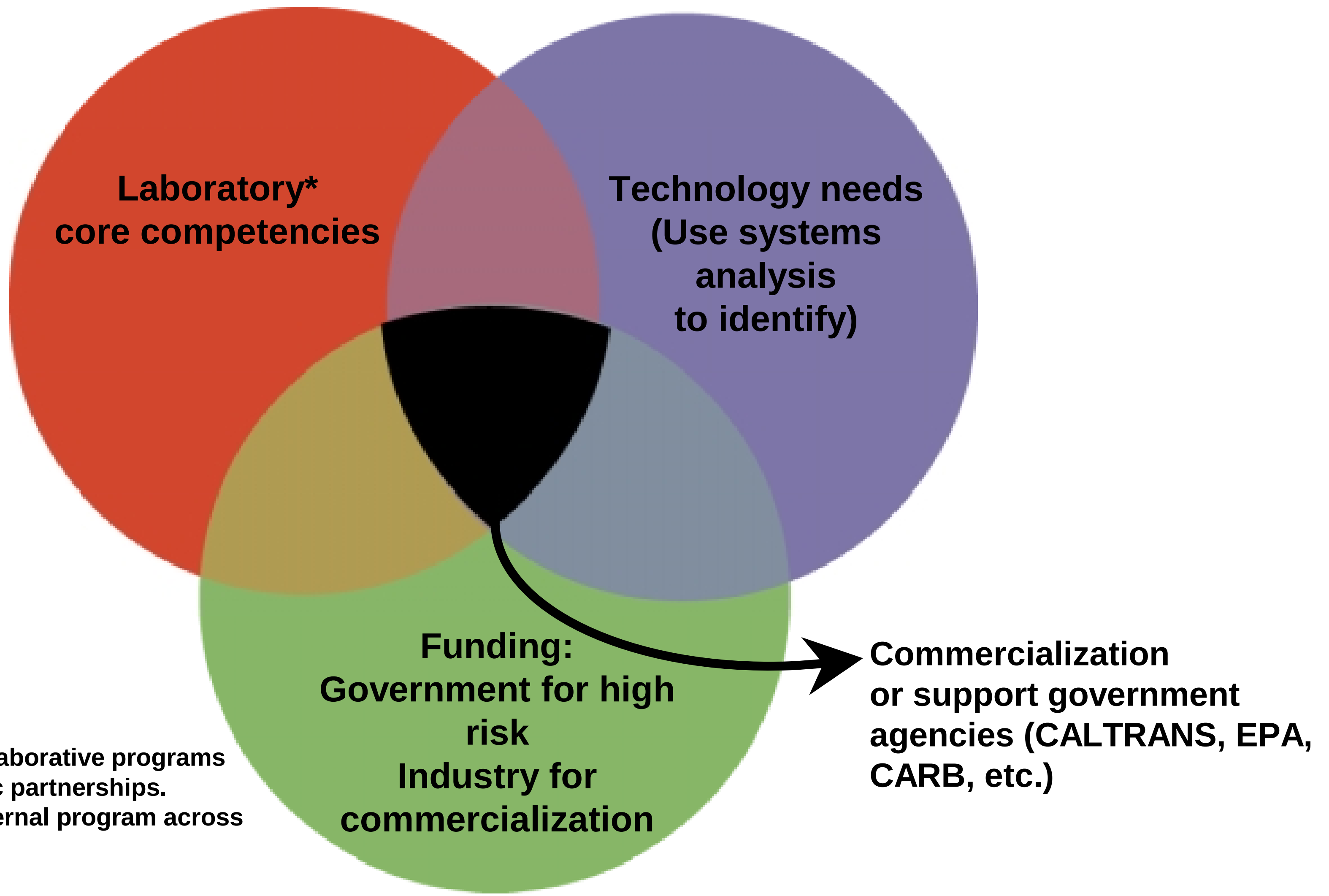
- **Employees**
  - LLNL: 7,250
  - Other: 750
- **Capital Plant: $4B**
- **Annual Operating and Capital funds: ~$1B/yr**

Managed by the University of California since 1952

Our strategy is to identify the intersection between lab core competencies, technology needs, and funding



* 1) Develop collaborative programs and strategic partnerships.
2) Integrate internal program across directorates.

Chemical Kinetic Model

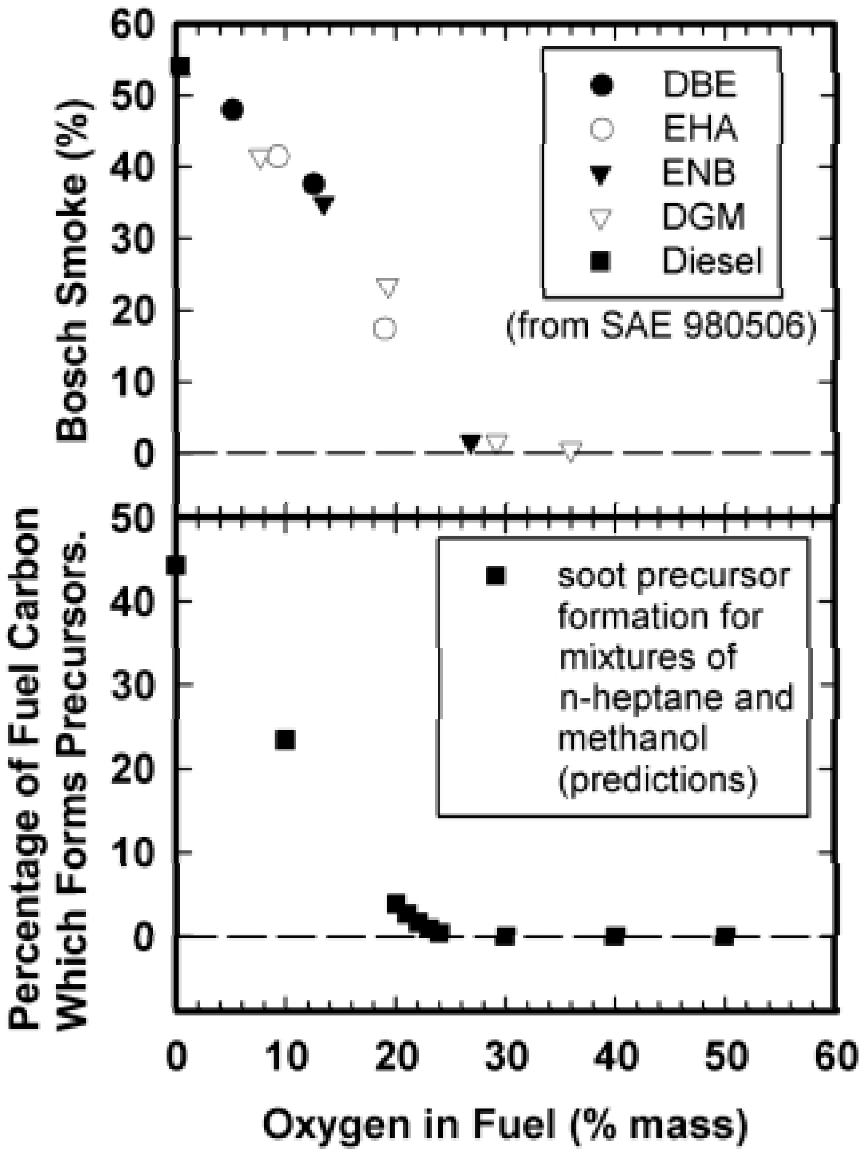
Contains a large database of:

- Thermodynamic properties of species
- Reaction rate parameters

Size of mechanism grows with molecular size:

Fuel:	H_2	CH_4	C_3H_8 (Propane)	C_6H_{14} (Hexane)	$C_{16}H_{34}$ (Cetane)
Number of species:	7	30	100	450	1200
Number of reactions:	25	200	400	1500	7000

Predicted level of soot precursors correlates well with soot emissions from a Diesel engine



Hydrocarbon kinetics at LLNL

Types of systems studied

Flames

Shock tubes

Detonations

Pulse combustion

Flow reactors

Stirred reactors

Supercritical water oxidation

Engine knock and octane sensitivity

Flame extinction

Diesel engine combustion

Combustion of metals

Homogeneous Charge,
Compression Ignition (HCCI)

Waste incineration

Kerogen evolution

Oxidative coupling

Heat transfer to surfaces

Static reactors

Ignition

Soot formation

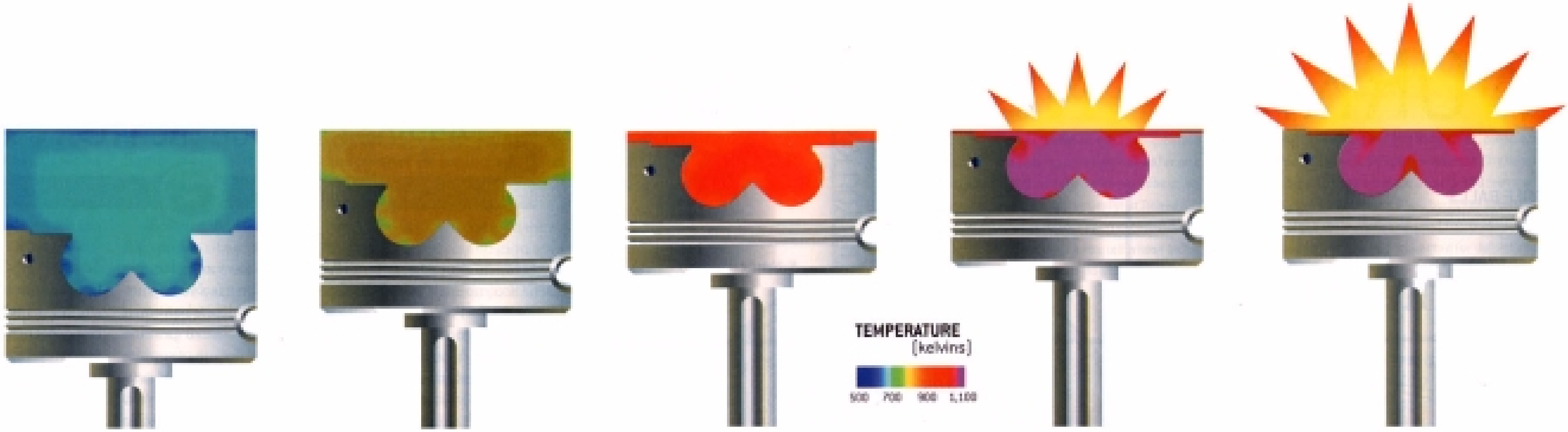
Pollutant emissions

Cetane number

Liquid fuel sprays

HE & propellant combustion

Homogeneous Charge Compression Ignition (HCCI) Engines



- Diesel engines are unlikely to achieve the NO_x and particulate matter levels required by future legislation

Potential of HCCI Engines

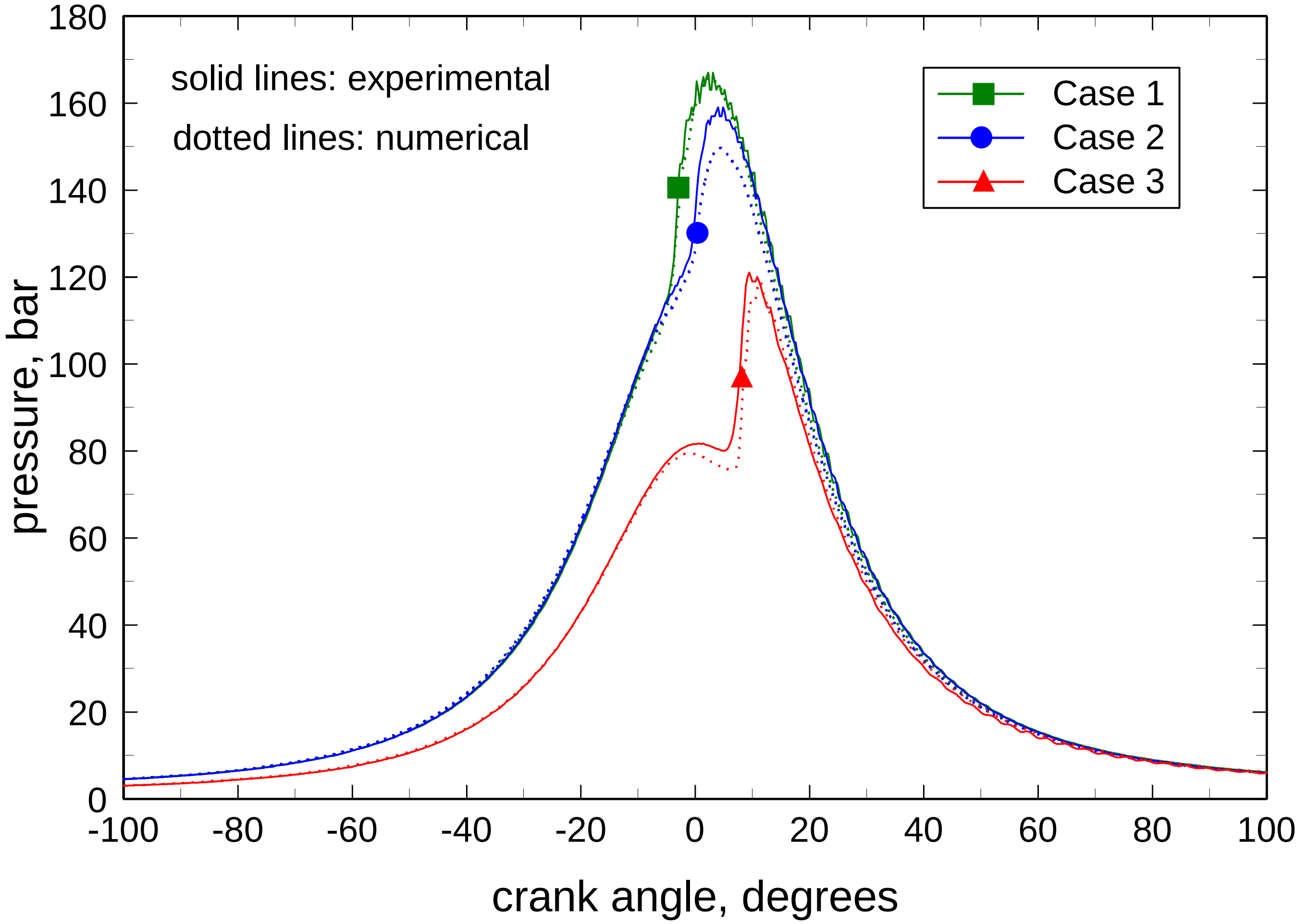
High efficiency
Very low NO_x
Low cost (no need for high pressure injection system, 1/3rd of engine cost)
Low cycle-to-cycle variation
Fuel flexibility
Unthrottled operation

Technical challenges of HCCI

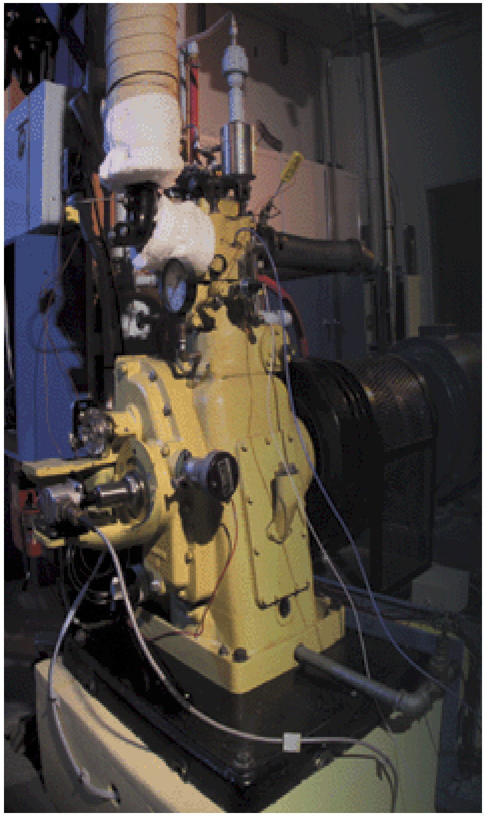
Difficult to control
Difficult to start
High peak heat release and peak pressure
High hydrocarbon and CO emissions

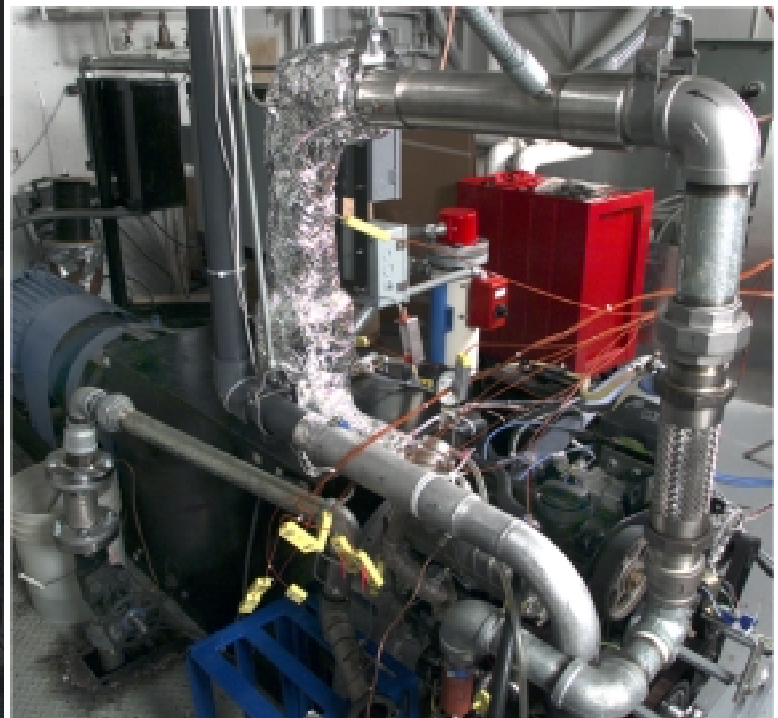
We have validated our multi-zone model with Cummins data for propane (SAE 2001-01-1027)

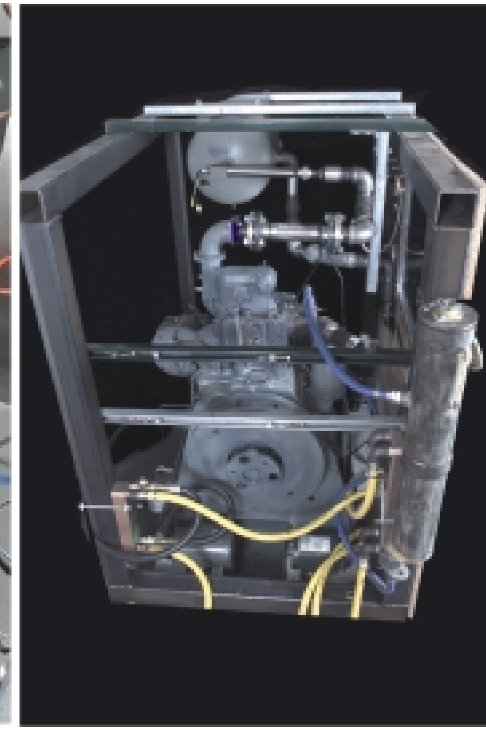
Case 1: 1002 rpm, ϕ=0.17, P_{in}=2.72 bar, T_{in}=352 K
Case 2: 1001 rpm, ϕ=0.17, P_{in}=2.75 bar, T_{in}=340 K
Case 3: 1800 rpm, ϕ=0.36, P_{in}=1.88 bar, T_{in}=342 K



We are working with three different HCCI experimental engines (a fourth engine has been donated by Ford)





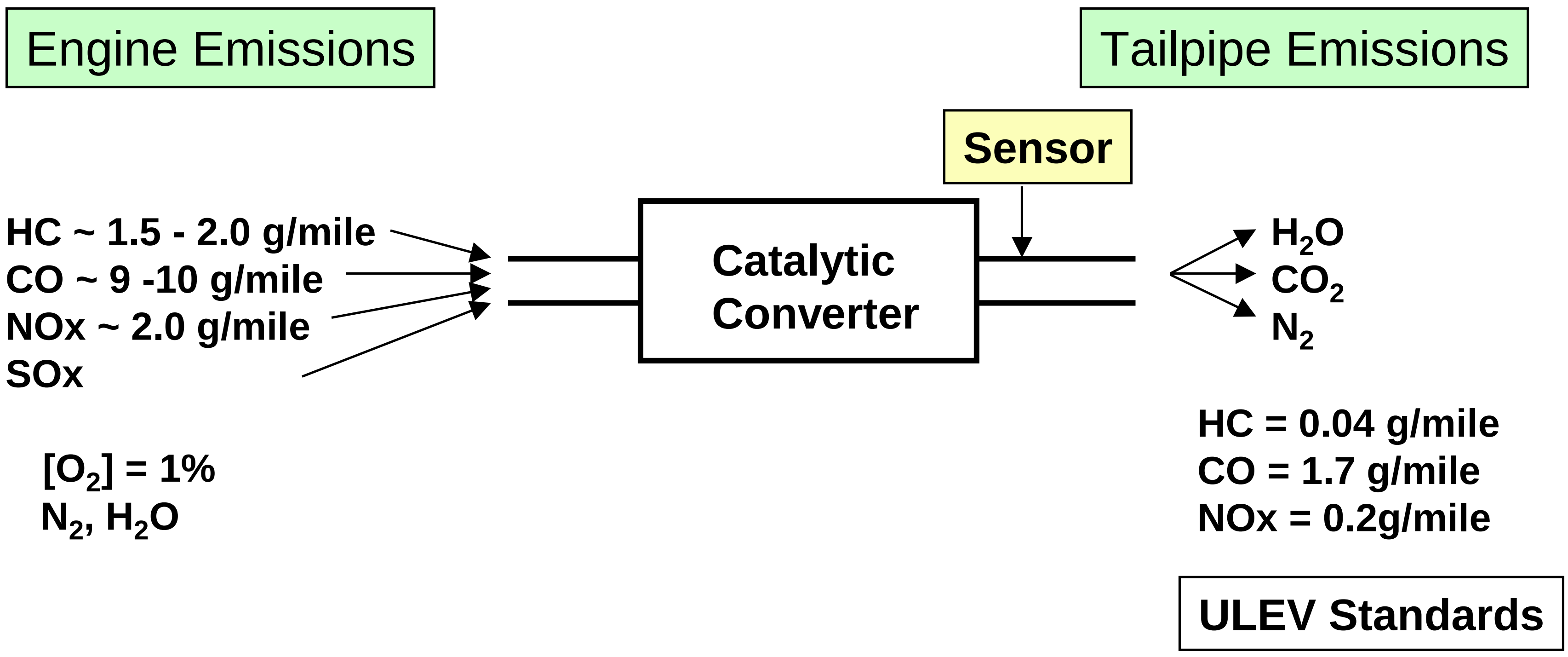


- CFR engine
- First experimental prototype

- Volkswagen TDI engine
- High-speed, 4-cylinder small displacement engine

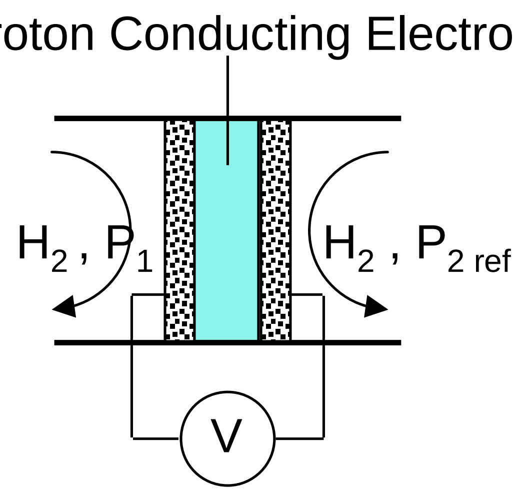
- Caterpillar 3401 engine
- Representative of heavy-duty diesel engines

Objective: Sensor for On-Board Monitoring of Catalytic Converter Performance



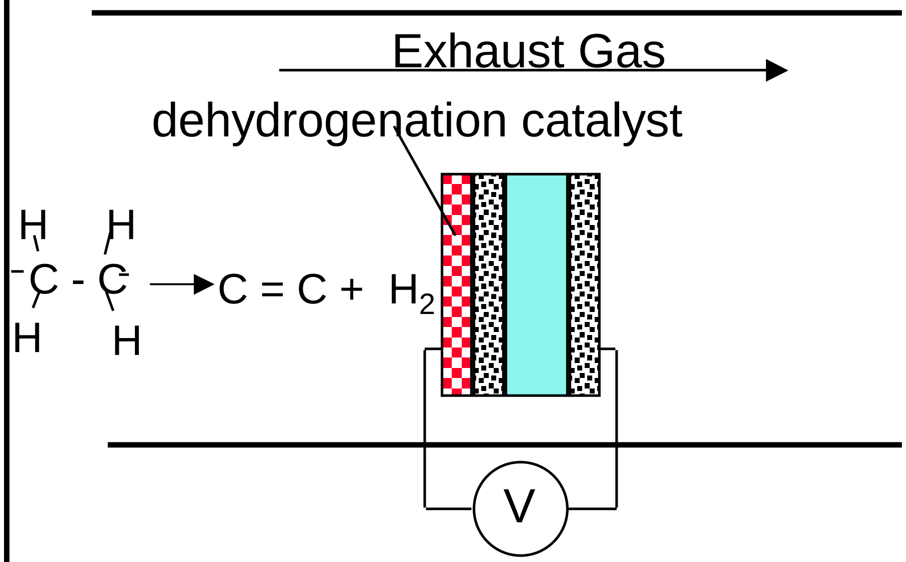
Principle of LLNL hydrocarbon sensor

Hydrogen Sensor



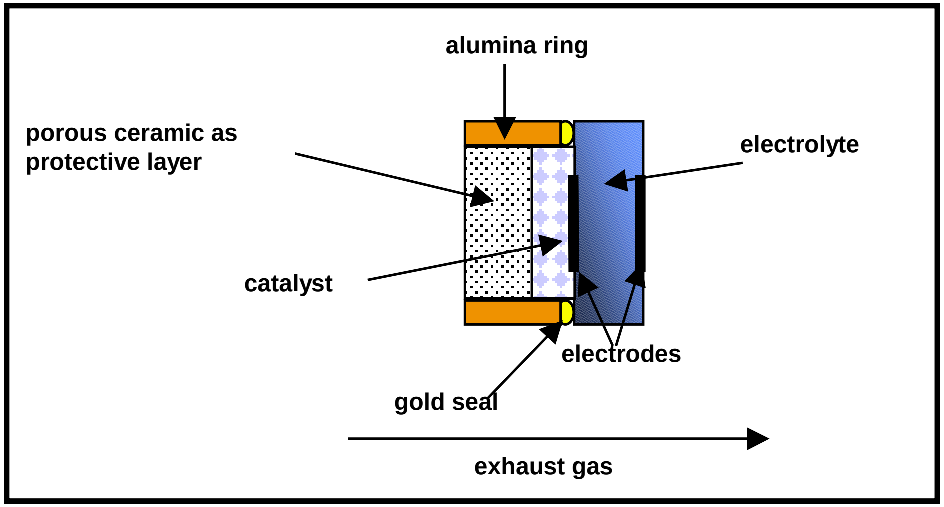
$$E = RT/nF \ln (P_1/P_2)$$

LLNL Hydrocarbon Sensor



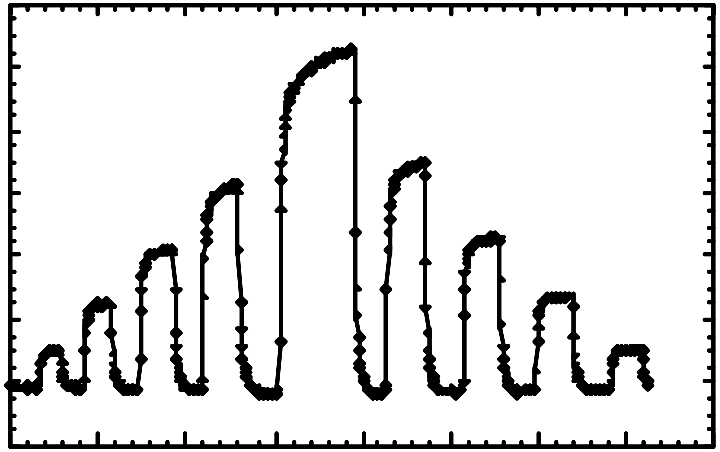
Possible Catalytic Reactions:
- dehydrogenation
- steam reforming
- cracking

Hydrocarbon sensors effort has put LLNL in forefront for future R&D from DOE/OTT



Applications

- Solid-state electrochemical sensors for monitoring hydrocarbons and NOx in engine exhaust



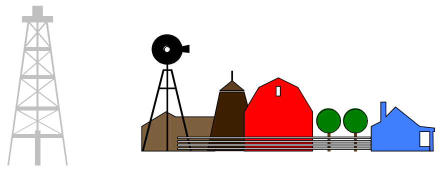
Accomplishments

- Dehydrogenation catalyst in combination with a proton-conducting electrolyte
- Demonstrated sensitivity to a variety of HCs with better than 25 ppm resolution
- Durability and sensitivity verified by Ford

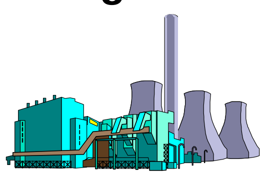
Center for Fuels Assessment: develop a system-based framework that addresses transportation fuel cycle

Fuel cycle

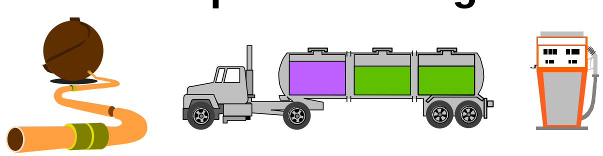
Exploration & production



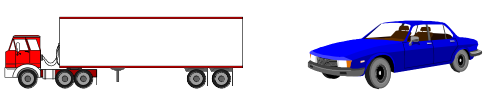
Reprocessing & refinement



Transport & storage



End-use



- Simulate and quantify contaminant releases to environment from fuel cycle components*
- Simulate contaminant dispersion in the environment*
- Estimate human exposure and associated health risk from environmental contaminants*
- Perform risk management*

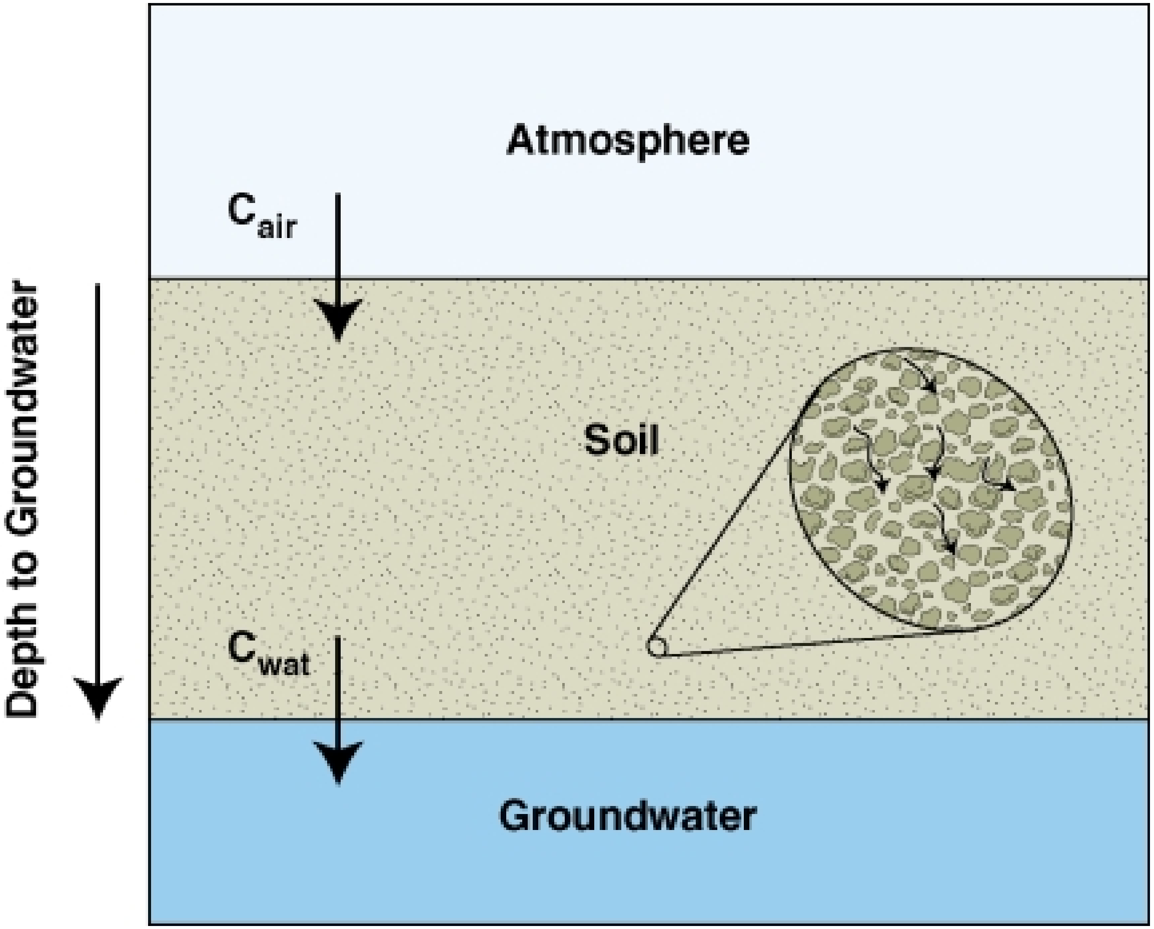
* Estimates will include both (1) individual fuel cycle component or (2) entire fuel cycle

Vulnerability of ground water to fuel compounds emitted to the atmosphere

- **Contaminant transport in soil occurs via diffusion in soil water and air and advection with infiltrating rainwater.**

- **Degradation occurs by both biotic and abiotic processes.**

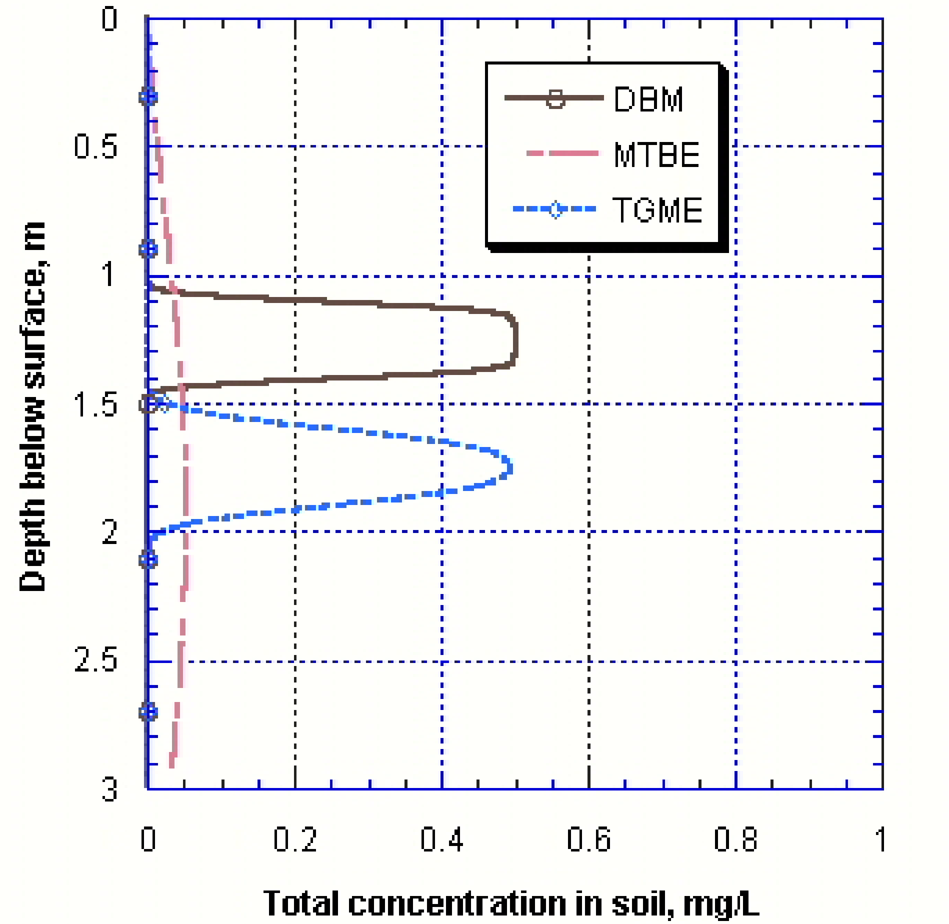
- **The contamination vulnerability of ground water to airborne releases of fuel compounds depends on soil and contaminant properties as well as transformation processes.**



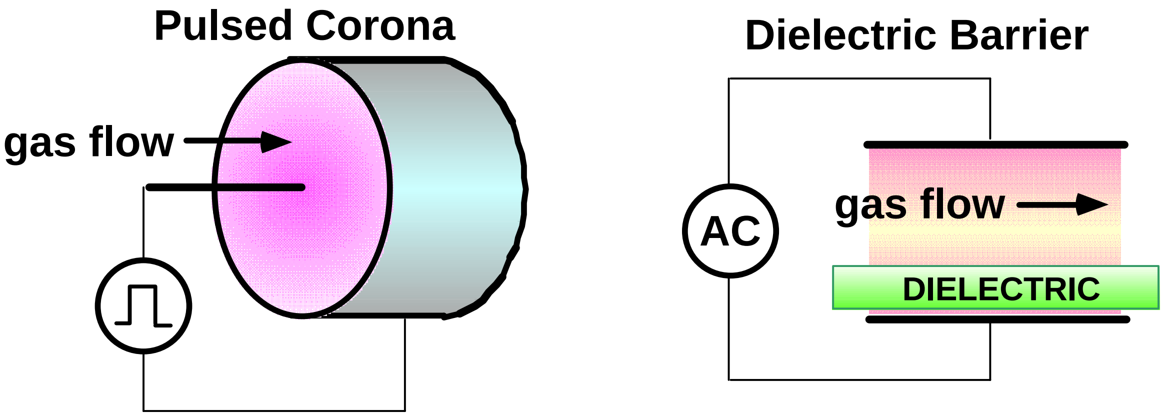
Concentration profiles of DBM, TGME, and MTBE in soil after 1 yr of transport from a buried source

Initial source is 1 m beneath the surface of a reference sandy soil and is uniformly contaminated to a depth of 30 cm.

- For this comparison, the compounds are again assigned a half-life of 1 year.
- Diffusion of MTBE in soil gas rapidly redistributes it through the soil column.
- TGME moves with infiltrating water (18 cm/yr), whereas DBM transport is retarded due to soil sorption.



Non-thermal plasmas can be used for the selective partial oxidation of NO to NO_2

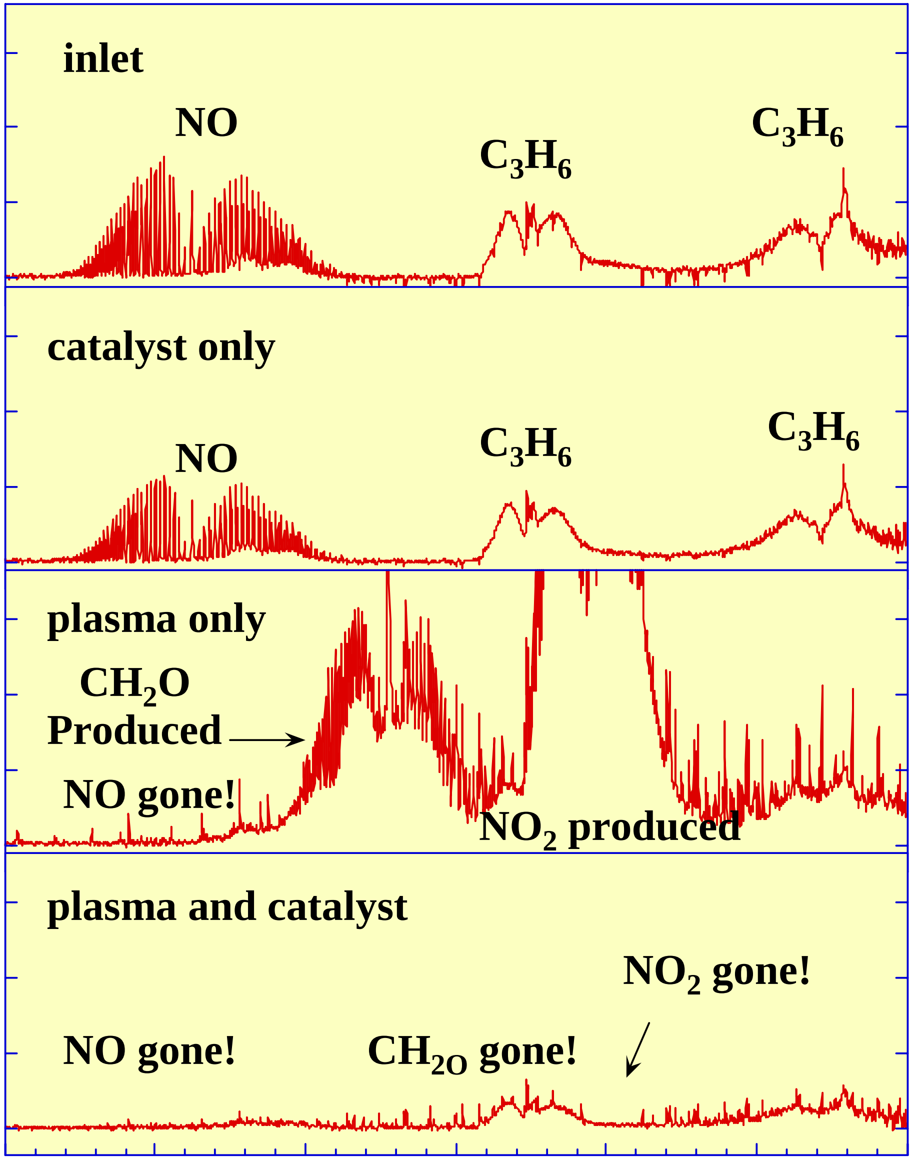


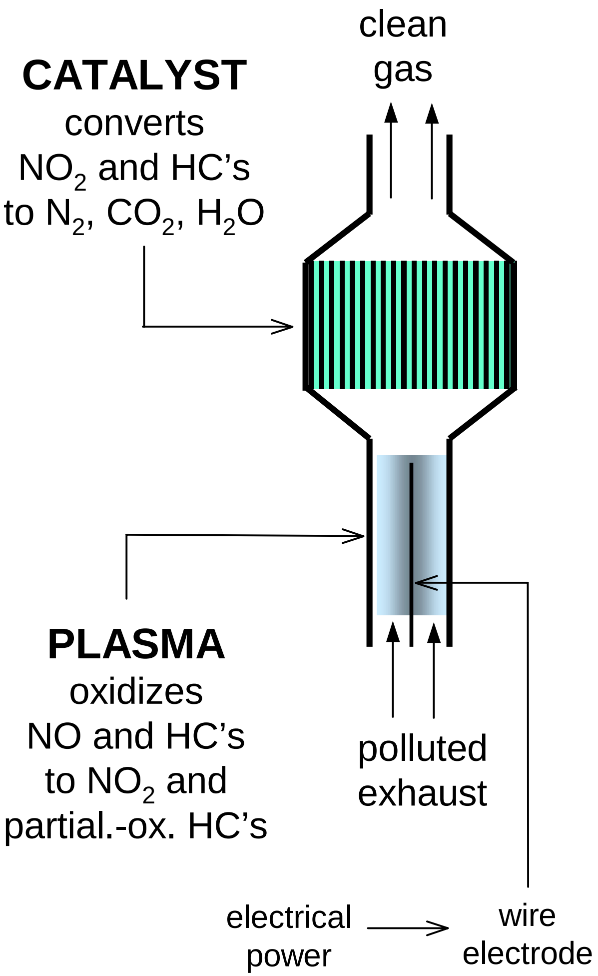
- Electrodes in atmospheric-pressure gas stream.
- High voltage is applied to accelerate the electrons.
- Hot electrons dissociate the background gas molecules to produce oxidizing radicals.

$$e + O_2 \rightarrow e + O(^3P) + O(^1D)$$

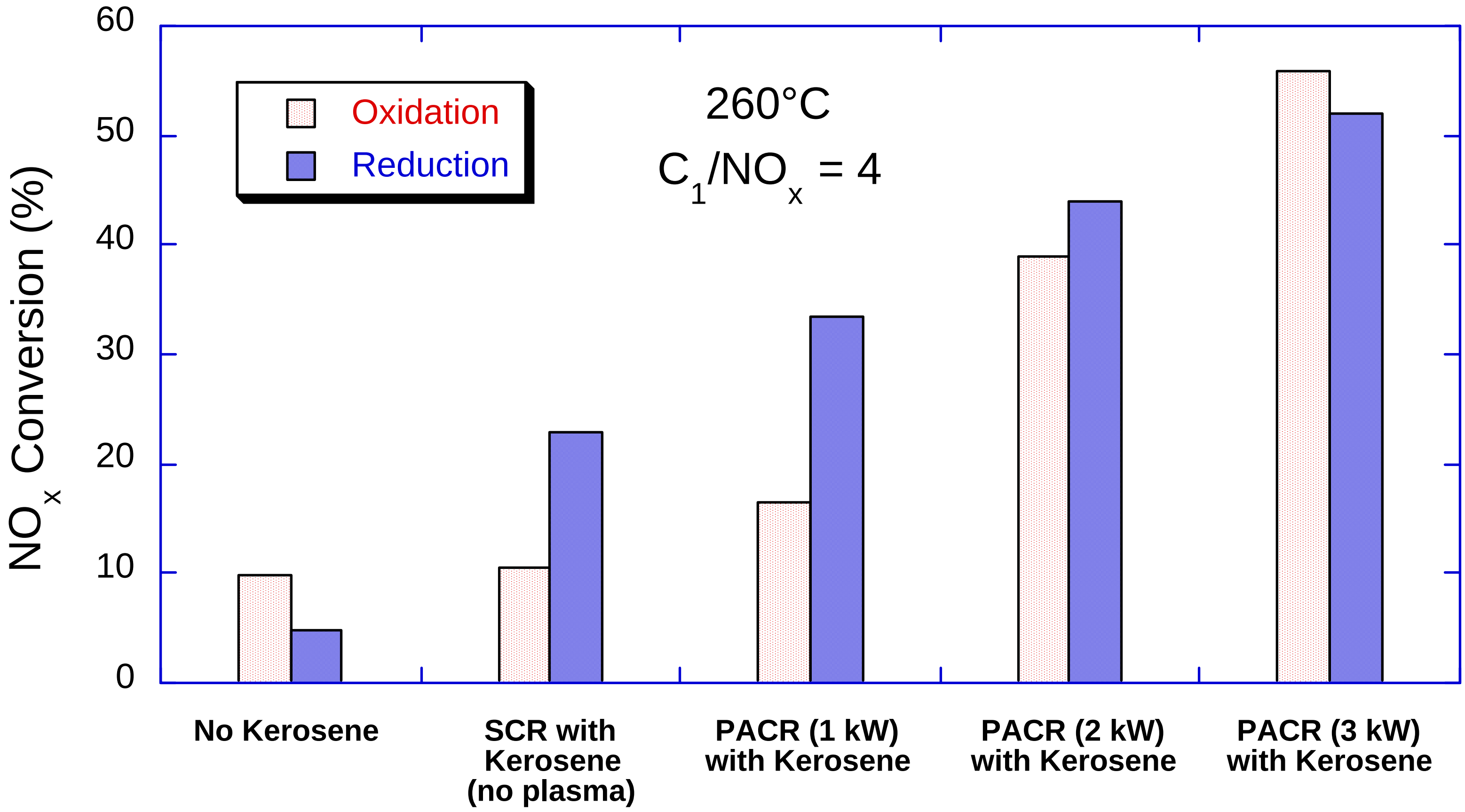
$$O(^3P) + NO \rightarrow NO_2$$

Plasma-Assisted Catalytic Reduction of NO_x





We have successfully done full-scale testing of the plasma/catalyst process on a Cummins 100 kW diesel engine



Using only 3% of the engine power output, the plasma increases the NO_x reduction efficiency of a cheap catalyst by more than 2x.

Other relevant LLNL engine technologies

- Magnetic bearings for turbochargers
- Isotopic tracing of fuel components
- InVest: Integrated Vehicle Simulation Environment Test bed
- Femptosecond Laser
- Laser peening